

Phenol, 2,5-dichloro, TMS

Other names: 2,5-Dichlorophenol, trimethylsilyl ether
Inchi: InChI=1S/C9H12Cl2OSi/c1-13(2,3)12-9-6-7(10)4-5-8(9)11/h4-6H,1-3H3
InchiKey: ZCUPEMVXIWKCSF-UHFFFAOYSA-N
Formula: C9H12Cl2OSi
SMILES: C[Si](C)(C)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 235.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	4.207		Crippen Method
rinpol	1359.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1356.20		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1356.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U325593&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/29-185-5/Phenol-2-5-dichloro-TMS.pdf>

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